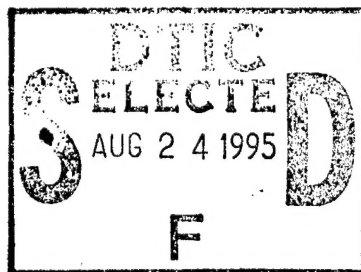


RADIATION ASSOCIATED WITH ATOMIC OXYGEN

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1 September 1995



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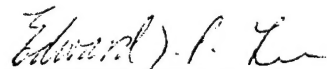
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Free-Free Transitions in Collisions between Slow Electrons
and Neutral Oxygen Atoms

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1. INTRODUCTION

During an encounter with an atom, an electron may emit (Bremsstrahlung) or absorb (inverse Bremsstrahlung) a photon in a manner that the atom is not affected energetically. Such free-free transitions of electrons are important source of emission and absorption processes in the stellar atmospheres and the low-temperature plasmas [1-3].

The free-free transitions with the neutral atomic oxygen as a host have been studied theoretically by several groups [4-7]. Since the free-free transitions assume a particular importance at low-incident electron energies, usually below the first excitation threshold, the target polarization is an important factor to consider in the theoretical calculation. Thus, in the work of Mjolsness and Ruppel [4] and of Geltman [5] an empirical polarization potential is included in the calculation of the continuum wave functions. John [6] obtained the absorption coefficients from the momentum-change cross sections by means of a formula suggested by Dalgarno and Lane [8]. Later John and Williams [7] adopted the multichannel theory of Morgan and John [9] to calculate the absorption coefficients, utilizing the results of a three-state close-coupling calculation of the electron-atom scattering [10].

In this work we account for the target polarization by means of the method of polarized orbitals which Temkin [11] devised to study the e-O scattering and later extended to the e-H problem [12]. Henry has also applied this method to study the elastic scattering of the e-O system and photodetachment from O^- [13]. In the polarized-orbitals method, the target polarization is made a part of the atomic wave functions which depend parametrically on the incident-electron coordinates. The polarized orbitals in turn present the (polarization) potential to the scattering electron. Thus, we are in a position to compare the results based on three different ways of handling the target polarization - by the empirical polarization potential, by the multi-state close-coupling, and by the method of polarized orbitals.

In Sec. 2, we briefly discuss the basic formulation of free-free absorption and emission coefficients, and describe the method by which the free-electron functions are obtained. The

polarized-orbitals method of Temkin, from which the polarization potentials are derived, is described in Sec. 3. A short description of the numerical procedure is contained in Sec. 4. In Sec. 5, we compare our results with the previous works in some detail, particularly with the work of John and Williams [7], since our approach and theirs may be viewed as complementary. Section 6 concludes this report.

2. THEORY

2.1 Absorption and Emission Coefficients

We study the free-free transition process

$$e^-(\vec{k}_i) + O(2p^4 \ ^3P) \rightarrow e^-(\vec{k}_f) + O(2p^4 \ ^3P) \pm \hbar\omega, \quad (1)$$

in which a photon is emitted ($+\hbar\omega$) or absorbed ($-\hbar\omega$). The conservation of energy gives the relationship

$$\frac{(k_i\hbar)^2}{2m} = \frac{(k_f\hbar)^2}{2m} \pm \hbar\omega. \quad (2)$$

It is appropriate to construct the wave functions of the (e^-+O) system that are eigenfunctions of the total orbital (L) and spin (S) angular momenta if we neglect the spin-orbit interaction. Then the transitions of interest are of the type

$$[2p^4(S_1L_1)k_i\ell SL] \rightarrow [2p^4(S_1L_1)k_f\ell' SL'], \quad (3)$$

where $S_1=L_1=1$ for the 3P state, and (ℓ, ℓ') are the partial waves of the incident and scattered electrons. The dipole matrix elements for the above transition have been worked out [16]. Using these results the formula for the absorption cross sections $\sigma_{abs}[1,2]$ can be generalized, viz.,

$$\sigma_{abs}(k_i, \Delta k^2) = \frac{256\pi^2\alpha a_o^5}{3k_i^2k_f(\Delta k^2)^3} M^2, \quad (4)$$

where α is the fine-structure constant,

$$\Delta k^2 = |k_i^2 - k_f^2|, \quad (5)$$

$$M^2 = \sum_{\ell'} \ell_{>} \left\{ \sum_{SLL'} \frac{(2S+1)}{2(2S_1+1)} \frac{(2L+1)(2L'+1)}{(2L_1+1)} W^2(\ell L \ell' L'; L_1 1) |M_{\ell, \ell'}^{LL'S}|^2 \right\}. \quad (6)$$

In the above $\ell_{>}$ is the greater of ℓ and ℓ' and W is the Racah coefficient, and

$$M_{\ell, \ell'}^{LL'S} = \int_0^\infty P_{k_i \ell}^{LS}(r) \frac{dV(r)}{dr} P_{k_f \ell'}^{L'S}(r) dr, \quad (7)$$

where $r^{-1}P_{k_i \ell}^{LS}(r)$ is the radial part of the continuum function of the free electron and $V(r)$ is the potential seen by the free electron. If the dependency of $M_{\ell, \ell'}^{LL'S}$ on (L, L', S) is suppressed, the quantity inside the curly bracketed in Eq. (6) reduces to $M_{\ell, \ell'}^2$, so that Eq. (4) reverts back to Eq. (6) of Ref. [2].

The (mean) absorption coefficient is obtained by averaging the cross sections over the Maxwellian distribution function $f(v, T)$ corresponding to the electron temperature T , viz.

$$\kappa(\lambda, T) = \int_0^\infty \sigma_{abs}(k_i, \Delta k^2) f(v_i, T) dv_i, \quad (8)$$

where

$$f(v, T) dv = \frac{4}{\sqrt{\pi}} \left(\frac{m}{2kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right) v^2 dv, \quad (9)$$

$$= 198.0 \Theta^{3/2} \exp(-31.3296 k_i^2) k_i d(k_i^2), \quad (10)$$

with

$$\Theta = 5040/T(K), \quad (11)$$

so that

$$\kappa(\lambda, T) = \frac{5.05 \times 10^{-39} \Theta^{3/2}}{(\Delta k^2)^3} \int_0^\infty \frac{\exp(-31.3296 k_i^2)}{k_i k_f} M^2 d(k_i^2). \quad (12)$$

The wavelength λ and Δk^2 are related as

$$\lambda(\text{\AA}) = 911.8/\Delta k^2(a.u.). \quad (13)$$

The cross sections in Eq.(4) are expressible in units of $\text{cm}^5[1]$ after a substitution of $a_0 = 0.529 \times 10^{-8} \text{cm}$, so that the absorption coefficients in Eq. (12) are also in units of

cm⁵. The absorption cross sections and coefficients are frequently multiplied by the electron density n that would give rise to a pressure of 1 dyne/cm² at temperature T ,

$$n(\text{cm}^{-3}) = 0.724 \times 10^{16}/T(K) \quad (14)$$

per dyne/cm² [1] so that the cross sections and coefficients are now expressible in cm⁴/dyne. The photons involved in the absorption also induce emission so that the absorption coefficients are sometimes multiplied by a factor $[1 - \exp(-h\nu/kT)]$ [1]. In this paper we do not include this factor unless specifically stated otherwise.

The expression of the emission cross sections has been given in Refs.[4,5]. However, a more pertinent quantity in applications is the emissivity in units of W-cm³/μm-steradian [5], which we found to be

$$J(\lambda, T) = \frac{0.794814 \times 10^{-31}}{[\lambda(\mu\text{m})]^2} \Theta^{3/2} \int_{v_o}^{\infty} \frac{\exp(-31.3296 \frac{k_i^2}{k_i k_f})}{k_i k_f} M^2 d(k_i^2), \quad (15)$$

where v_o is the threshold velocity of the free electron for emission, i.e.,

$$\frac{1}{2}mv_o^2 = \hbar\omega \quad (16)$$

and the symbol $\lambda(\mu\text{m})$ indicates that λ is to be expressed in μm. The emissivity in this work was computed by Eq. (15). Geltman [5] also gave the relationship

$$J(\lambda, T) = \frac{1.19 \times 10^4}{[\lambda(\mu\text{m})]^5} \exp\left(-\frac{1.439 \times 10^4}{\lambda(\mu\text{m})T}\right) \kappa(\lambda, T), \quad (17)$$

which can be used to check the consistency between Eqs.(12) and (15).

2.2 Free Electron Function $P_{kl}^{LS}(r)$

The reduced radial function $P_{kl}^{LS}(r)$ is obtained as the solution of the integro-differential equation

$$\begin{aligned} & \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V_{Coul}^L(r) - V_{pol}^L(r) + k^2 \right] P_{kl}^{LS}(r) \\ & = \sum_{n'\ell'\lambda} W_{n'\ell'\lambda, kl}^{LS} P_{n'\ell'}(r) + \sum_{n'\ell'} \delta_{\ell'\ell} C_{n'\ell'} P_{n'\ell'}(r), \end{aligned} \quad (18)$$

where V_{Coul}^L and V_{pol}^L are the Coulomb potential due to the unperturbed atomic orbitals and the polarization correction (to be discussed in Sec. 3) respectively. The first term on the RHS is the exchange interaction term and the second term is to ensure the orthogonality with the bound atomic orbitals \mathcal{P}_{nl} . The dependency on the angular momenta L and S is indicated as superscripts.

With regard to the present problem of $O^- [1s^2 2s^2 2p^4 ({}^3P) k\ell {}^{2,4}L]$, the unperturbed orbitals of the oxygen atom are

$$\phi_{nlm}^o(\vec{r}) = Y_{lm}(\hat{r}) r \mathcal{P}_{nl}(r), \quad (19)$$

and the Coulomb potential is

$$\begin{aligned} V_{Coul}^L(r) = 2 \left\{ -\frac{Z}{r} + 2y_o(1s, 1s|r) + 2y_o(2s, 2s|r) \right. \\ \left. + 4y_o(2p, 2p|r) + \frac{1}{5}v_2^L y_2(2p, 2p|r) \right\}, \end{aligned} \quad (20)$$

where Z is the nuclear charge, and

$$\begin{aligned} y_\lambda(n\ell, n'\ell'|r) = r^{-\lambda-1} \int_0^r \mathcal{P}_{nl}(t) \mathcal{P}_{n'\ell'}(t) t^\lambda dt \\ + r^\lambda \int_r^\infty \mathcal{P}_{nl}(t) \mathcal{P}_{n'\ell'}(t) t^{-\lambda-1} dt, \end{aligned} \quad (21)$$

and v_2^L is equal to $\ell/(2\ell+3)$, -1 , and $(\ell+1)/(2\ell-1)$ for $L=\ell+1$, ℓ , $\ell-1$ respectively.

The exchange terms are

$$\begin{aligned} \sum_{n'\ell'\lambda} W_{n'\ell'\lambda, k\ell}^{LS}(r) \mathcal{P}_{n'\ell'}(r) = 2 \left\{ -\frac{1}{2\ell+1} y_\ell(1s, k\ell|r) \mathcal{P}_{1s}(r) \right. \\ - \frac{1}{2\ell+1} y_\ell(2s, k\ell|r) \mathcal{P}_{2s}(r) + w_{\ell+1}^{LS} y_{\ell+1}(2p, k\ell|r) \mathcal{P}_{2p}(r) \\ \left. + w_{\ell-1}^{LS} y_{\ell-1}(2p, k\ell|r) \mathcal{P}_{2p}(r) \right\}, \end{aligned} \quad (22)$$

where $y_\ell(n\ell, k\ell|r)$ can be obtained from Eq.(21) by substituting $\mathcal{P}_{k\ell}^{LS}(t)$ for $\mathcal{P}_{n'\ell'}(t)$.

The coefficients w_λ^{LS} are shown in Table 1. Throughout the work, we have used the wave functions of Clementi and Roetti [17] for the unperturbed orbitals. Finally, Eq. (18) is to be solved subject to the boundary condition,

$$\lim_{r \rightarrow \infty} P_{k\ell}^{LS}(r) = \sin(kr - \frac{1}{2}\ell\pi + \eta_{k\ell}^{LS}), \quad (23)$$

where η_{kl}^{LS} is the phase shift due to interaction with the atom.

Determination of the polarization potential $V_{pol}^L(r)$ in Eq.(18) will be taken up in Sec. 3. At this point we should note that if we drop the $V_{pol}^L(r)$ term, then Eq.(18) becomes a "one-channel" closing-coupling equation obtainable by omitting all coupling terms connecting the different partial waves and the various target-atom states. The polarization potential may be viewed as a way to account for the effects of the omitted channels on the free-electron wave function. This may be contrasted with the work of John and Williams [7] in which they used the results of a three-state close-coupling calculation with no explicit introduction of the polarization potential as the inclusion of the coupling channels in their work is another way to allow for the target polarization.

3. METHOD OF POLARIZED ORBITALS

In this section we briefly recall the essential steps in Temkin's method of polarized orbitals [11], ultimately leading to the polarization potential $V_{pol}^L(r)$ in Eq. (18). The details are found in the works of Temkin and others [11-13]. Here the distortion of the target atom caused by the perturbation of the free electron at \vec{r}_{N+1} is treated in an adiabatic, dipole approximation with the proviso that the perturbing electron is outside the atomic electrons. Thus the perturbation is taken as

$$H' = \left(\frac{4\pi}{3}\right) \frac{1}{r_{N+1}^2} \sum_{i=1}^N r_i \epsilon(r_i, r_{N+1}) \sum_{\mu=-1}^1 Y_{1\mu}^*(\hat{r}_i) Y_{1\mu}(\hat{r}_{N+1}), \quad (24)$$

$$\epsilon(r_i, r_{N+1}) = \begin{cases} 1, & \text{for } r_{N+1} \geq r_i \\ 0, & \text{for } r_{N+1} < r_i. \end{cases} \quad (25)$$

To construct the wave function of $O(^3P)$ we start with the unperturbed one-electron functions of the oxygen atom [17] as shown in Eq.(19). Following Temkin we add a polarization correction to each ϕ_{nlm}^o to form a polarized orbital which depends parametrically on \vec{r}_{N+1} as

$$\phi_{nlm}(\vec{r}, \vec{r}_{N+1}) = \phi_{nlm}^o(\vec{r}) + \lambda \phi_{nlm}^{cor}(\vec{r}, \vec{r}_{N+1}), \quad (26)$$

$$\lambda \phi_{nlm}^{cor}(\vec{r}, \vec{r}_{N+1}) = \varepsilon(r, r_{N+1}) \sum_{\ell'm'} Y_{1,m-m'}(\hat{r}_{N+1}) \phi'_{nlm \rightarrow \ell'm'}(\vec{r}). \quad (27)$$

It is convenient to define

$$\phi'_{nlm \rightarrow \ell'm'}(\vec{r}) = c(\ell m \rightarrow \ell' m') Y_{\ell'm'}(\hat{r}) r P_{nlm \rightarrow \ell'm'}(r), \quad (28)$$

where

$$c(\ell m \rightarrow \ell' m') = 2(-1)^{m'-m} \left[\frac{4\pi(2\ell+1)}{(2\ell'+1)} \right]^{1/2} c(1 m' - m \ell m; \ell' m') c(1 0 \ell 0; \ell' 0). \quad (29)$$

In the above $c(j_1 m_1 j_2 m_2; j m)$ is the Clebsch-Gordan coefficient; thus, we see that $|\ell' - \ell| = 1$ and $|m' - m| = 0, 1$.

The radial function $P_{nlm \rightarrow \ell'm'}(r)$ is obtained as the solution of the differential equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell'(\ell'+1)}{r^2} - V'_{Coul}(r) + E_{nl} \right] P_{nlm \rightarrow \ell'm'}(r) = \sum_{n''\ell''\lambda} W'_{n''\ell''\lambda, \ell'm'}(r) P_{nlm \rightarrow \ell'm'}(r) + \sum_{n''\ell''} \delta_{\ell''\ell'} C_{n''\ell''} P_{n''\ell''}(r) + r P_{nl}(r). \quad (30)$$

Here the Coulomb (V'_{Coul}) and exchange (W') potentials are obtainable by subjecting to the Hartree-Fock procedure the determinantal wave functions in which the parent orbitals $\phi_{nlm}^o(\vec{r})$ are replaced by the polarized version of Eq. (26). The function $P_{nlm \rightarrow \ell'm'}(r)$ approaches zero as $r \rightarrow \infty$, and for small r

$$\lim_{r \rightarrow 0} P_{nlm \rightarrow \ell'm'}(r) = ar^{\ell'+1}. \quad (31)$$

In this work we have obtained the $P_{nlm \rightarrow \ell'm'}$ functions associated with the unperturbed orbitals $nl=2s$ and $2p$. For later reference, they are listed in Table 2, and are referred to simply as P_i therein. From these polarized orbitals we obtained the dipole polarizability of $5.084 a_0^3$ compared with the experimental value of 5.2 ± 0.4 [18]. Other theoretical values range from 4.63 to 5.41 [19]. In general the polarized orbitals $P_{nlm \rightarrow \ell'm'}$ depends on m and m' as well as on ℓ and ℓ' due to the difference in exchange term in Eq. (30) so that only two

pairs are identical among the fifteen functions in Table 2; that is, P_5 and P_6 , and P_{10} and P_{12} . This dependency on m and m' manifests itself, for example, in the calculation of dipole polarizability in which a difference up to 20% is found in the matrix elements.

When the target wave functions are described by the unperturbed orbitals ϕ^o , the Coulomb potential $V_{Coul}^L(r)$ seen by the free electron (coordinate \vec{r}), consists of constituent terms due to all occupied $n'\ell'$ -orbitals such as

$$v_{n'\ell'}(r) = \int Y_{\ell m}^*(\hat{r}) Y_{\ell m}(\hat{r}) |\vec{r} - \vec{r}'|^{-1} \phi_{n'\ell'}^{o*}(\vec{r}') \phi_{n'\ell'}^o(\vec{r}') d\vec{r}' d\hat{r}. \quad (32)$$

As a consequence of the polarization of the $n'\ell'$ -orbital, augmentation of the target orbitals by the polarization correction $\lambda \phi_{n\ell m}^{cor}$ in accordance with Eqs. (26) and (27) produces additional (polarization) terms, to the first order in λ , of the form

$$v_{n'\ell'm' \rightarrow \ell''m''}(r) = \int Y_{\ell m}^*(\hat{r}) Y_{\ell m}(\hat{r}) |\vec{r} - \vec{r}'|^{-1} \phi_{n'\ell'}^{o*}(\vec{r}') \phi'_{n'\ell'm' \rightarrow \ell''m''}(\vec{r}') d\vec{r}' d\hat{r}. \quad (33)$$

The polarization potentials associated with the Coulomb interaction which can be derived variationally [11] are composed of a series of such integrals, and can be cast into the general form

$$V_{pol}^L(r) = -\frac{2}{r^4} \sum_j C_j F_{u(j)}(\ell) \int_0^r \mathcal{P}_j(t) P_{B(j)}(t) t dt. \quad (34)$$

The notation used here requires some explanation. We have a summation over j which ranges from 1 to 15 for $L=\ell+1$, 1 to 21 for $L=\ell$, and 1 to 31 for $L=\ell-1$ as shown in Table 3. For each value of j , we also list C_j , $u(j)$, \mathcal{P}_j , and $B(j)$ in Table 3 for the three possible choices of $L=\ell+1$, ℓ , and $\ell-1$. To identify $P_{B(j)}$ let us take an example of, say, $j=5$ with $L=\ell+1$. The associated $B(j)$ is 7 according to Table 3. We then go to the entry of $i=7$ in Table 2 and find that $P_{B(j=5)}$ is $P_{2p,1 \rightarrow 2,2}$. From Table 4, we find $F_{u(j)}$ for each j in a similar way. \mathcal{P}_j is the reduced radial function of the unperturbed target orbitals as defined in Eq.(19) with $\mathcal{P}_j = \mathcal{P}_{2s}$ for $j \leq 3$ and $\mathcal{P}_j = \mathcal{P}_{2p}$ for $j > 3$.

The exchange potential is also modified by the inclusion of polarization. The effects of the polarization on the exchange term have been examined by Henry [13] in his work on the

elastic scattering of electron from the oxygen atom. The inclusion of this exchange term was found to change the s-wave ($\ell=0$) cross sections by only 10%. For the higher partial waves ($\ell > 0$), the difference is even smaller (4%) so that the influence of the polarization of the orbitals via exchange is seen to be rather marginal. For this reason, we do not consider in this paper the polarization correction on the electron exchange.

4. NUMERICAL PROCEDURES

The integro-differential equations of Eqs. (18) and (30) are solved non-iteratively by using the Lagrange-multiplier technique as we have done previously [20]. The inhomogeneity terms, which arise due to the electron exchange, orthogonality, and perturbation, are set to zero after $r=13.5 a_o$. This corresponds to the r value at which 2p function has decreased to 10^{-5} of its peak value. At this point the Lagrange multipliers are determined, and the complete solution is constructed as a linear combination of the particular integrals and homogeneous solution. Beyond $r=13.5 a_o$ Eqs. (18) and (30) are considered to be homogeneous differential equations.

For the free-electron functions, the phase shift η is determined at various points 50 to $250a_o$ apart starting at $450a_o$, until two successive values agree within 0.01%. To solve for the polarization correction functions of Eq. (30), the numerical solution is first initiated with a certain arbitrary value of a in Eq. (31). The resulting solution obtained by numerical integration in general would diverge at large r , say, tending to $+\infty$ as $r \rightarrow \infty$. The value of a used here is denoted by a_+ . We then change the value of a until the resulting solution tends to $-\infty$ at large r , and this new choice of a is denoted by a_- . By successive interpolation between a_+ and a_- , we develop a numerical solution for $P_{nlm \rightarrow l'm'}(r)$ that monotonically decreases up to $r=20a_o$.

The dipole matrix elements are computed by the velocity form instead of the acceleration form shown in Eq. (7). The length and acceleration forms may be derived from and is equivalent to the velocity form if the wave functions are exact eigenfunctions of the atomic Hamiltonian. Using a short-hand notation of $\gamma = (\text{LSk}\ell)$, we have

$$M_{\ell,\ell'}^{LL'S} = \frac{(\Delta k^2)a_o}{2} \int_0^\infty P_\gamma(r) \left[\frac{d}{dr} + \frac{\ell_>(\ell' - \ell)}{r} \right] P_{\gamma'}(r) dr, \quad (35)$$

where $\ell_>$ is the greater of ℓ and ℓ' . The limits of integral $(0,\infty)$ is divided into two regions $(0,R)$ and (R,∞) where R is the value of r at which the asymptotic form of Eq. (22) sets in. The integration in the interval $(0,R)$ is carried out numerically. For the interval (R,∞) , the integrals are expressed in closed forms analogous to those given in Ref. [21].

Using our computational procedures, we obtain virtually identical results for various entries in Tables 3 and 5 of Ref. [2]. In these calculations the difference between the velocity and acceleration forms was typically 1.5% or less.

5. RESULTS

In Eq. (6) we have $L_1 = S_1=1$ for the present problem (^3P ground state of O atom), and S takes on $1/2$ and $3/2$. We have also set the limit of $(\ell,\ell') \leq 4$, and (L, L') to all values consistent with (ℓ,ℓ') . For a given value of the wavelength λ (equivalently, of Δk^2), we have computed the cross sections at 200 different values of incident-electron energy from 0 to 1.2 a.u. as shown in Table 5. The process of averaging over the Maxwell-Boltzmann distribution in Eqs. (12) and (15) was carried out by interpolating between these 200 points. The resulting continuous absorption coefficients in Eq. (12) are shown in Table 6 and emissivity coefficients of Eq. (15) in Table 7.

Geltman [5] made an extensive calculation of the free-free absorption coefficients for a number of neutral-atom systems including the oxygen atom. A Hartree-Fock-Slater-type

potential was used to describe the Coulomb and exchange interaction of the free electron with the neutral atom, and an empirical polarization potential was added. The matrix elements are then evaluated in the acceleration form. At 10,000K, Geltman's values are 25-30% smaller than our values as shown in Table 8. A more detailed comparison of Table 4 of Ref. [5] and Table 6 of the present report shows that the coefficients in Ref. [5] are smaller than the present values at the lower electron temperatures and longer wavelengths of the absorbed photon. At higher temperatures the difference becomes smaller and at 20,000K the two sets are nearly identical. John [6] derived the free-free absorption coefficients involving various atoms and molecules from the momentum-loss cross sections by means of the formula suggested by Dalgarno and Lane [8]. The data of John for oxygen [6] are reported to be in good agreement with those of Geltman [5], particularly for $\lambda > 1.0\mu$.

A new and refined theoretical treatment was subsequently offered by John and Williams [7] in which they applied the multichannel theory [9] to obtain the free-free absorption coefficients for the e-O scattering system. For the continuum orbitals they used the scattering data from the three-state (3P , 1D , 1S of the ground configuration) close-coupling calculation of Saraph [10]. The bound states were described by the three-configuration wave functions. In Table 8, we compare their absorption coefficients at 9,700K, computed by the velocity form, with ours at 10,000K. In making this comparison two points should be mentioned. First, we estimate our absorption coefficients at 9,700K to be only about 3% smaller than the ones at 10,000K shown in Table 8. Secondly, the coefficients of John and Williams contain the contributions from cases other than the oxygen atom being in the ground 3P state before and after the collision. However, the 3P - 3P contribution is expected to occupy greater than 90% of the total at 9,700K, since its percentage is 90% at 12,600K and 99% at 5,040K (See Table 3 of Ref. [7]). Thus, even after accounting for the other contributions, the absorption coefficients of this work and of Ref. [7] differ by no more than 10% at 10,000K. In Table 5 of Ref. [7], John and Williams also give the absorption coefficients that include the factor for the stimulated emission. In Table 8 of this report we include their values at 5,040K,

adjusted so as to exclude the stimulated-emission factor and to be expressible in units of cm^5 . These values are seen to be about 10% smaller than our interpolated counterparts at 5,000K. Thus, the agreement is quite good. Furthermore, the percentage difference is about the same over a wide range of λ and at two different electron temperatures. This is encouraging and significant, because the two formalisms - the close-coupling method and the method of polarized orbitals - offer different approaches to allow for the effect of target polarization in a slow-electron-atom collision. This agreement may be contrasted with the comparison of the present calculation with that of Ref. [5], in which not only greater differences are found, but also the differences depend on λ and T .

From a shock-heated plasma experiment Taylor and Caledonia [14] obtained the absorption coefficients, which are shown in Table 8 as "Expt". In a similar experiment Kung and Chang [15] found the absorption coefficients of 7.8×10^{-38} and $3 \times 10^{-36} \text{cm}^5$ for $\lambda = 3.1$ and 9.85μ respectively, both at the electron temperature of 9700K. Those experimental values are about 2 to 3 times larger than the present values and those of Ref. [7]. Beyond the obvious difficulties associated with the experiments that are discussed in Refs. [14] and [15], we can offer no clear explanation for the discrepancy between the experiment and theory.

6. CONCLUSIONS

In an electron-atom collision the polarization of the target atom is an important and yet difficult feature to incorporate into the theoretical formalism. The multi-channel close-coupling method is one of the major theoretical tools that allow for the distortion of the target by the incident electron. In this paper we approached the same problem of the target polarization with the method of polarized orbitals. We found that this method gives the dipole polarizability of $5.084 a_0^3$ that is quite comparable to the range of values 4.63 to 5.41 by other calculations [19].

With respect to the free-free absorption coefficients our values show very good agreement (about 10%) with the results of John and Williams [7] based on the scattering data from a three-state close-coupling calculation. This agreement is significant in view of the very different nature between our approach and that of John and Williams. On the other hand the theoretical absorption coefficients are smaller by a factor of about two or three compared to the experimental values, and we are not able to reconcile this discrepancy at the present time.

Table 1. Values of w_{λ}^{LS} in Eq. (21).

S	L	w_{λ}^{LS}	
		$\lambda = \ell + 1$	$\lambda = \ell - 1$
$\frac{3}{2}$	$\begin{Bmatrix} \ell+1 \\ \ell \\ \ell-1 \end{Bmatrix}$	$-\frac{3(\ell+1)}{(2\ell+1)(2\ell+3)}$	$-\frac{3\ell}{(2\ell-1)(2\ell+1)}$
$\frac{1}{2}$	$\ell + 1$	$\frac{3\ell(2\ell+5)}{2(2\ell+1)(2\ell+3)^2}$	$-\frac{3\ell}{(2\ell-1)(2\ell+1)}$
$\frac{1}{2}$	ℓ	$\frac{3(\ell-2)}{2(2\ell+1)(2\ell+3)}$	$\frac{3(\ell+3)}{2(2\ell-1)(2\ell+1)}$
$\frac{1}{2}$	$\ell - 1$	$-\frac{3(\ell+1)}{(2\ell+1)(2\ell+3)}$	$\frac{3(2\ell-3)(\ell+1)}{2(2\ell-1)^2(2\ell+1)}$

Table 2. Polarized corrections $P_{n\ell m \rightarrow \ell' m'}$ that are equivalently referred to simply as P_i .

i	$n \ell, m \rightarrow \ell', m'$		i	$n \ell, m \rightarrow \ell', m'$	
1	2s,0	1,1	9	2p,1	2,0
2	2s,0	1,0	10	2p,0	2,1
3	2s,0	1,-1	11	2p,0	2,0
4	2p,1	0,0	12	2p,0	2,-1
5	2p,0	0,0	13	2p,-1	2,0
6	2p,-1	0,0	14	2p,-1	2,-1
7	2p,1	2,2	15	2p,-1	2,-2
8	2p,1	2,1			

Table 3. List of constituent parts that describe the polarization potential $V_{pol}^L(r)$ in Eq. (34).

j	C_j	$u(j)$	\mathcal{P}_j	B(j)
$L = \ell + 1$				
1	4/3	1	2s	1
2	4/3	2	2s	2
3	4/3	1	2s	3
4	4/3	1	2p	4
5	8/5	1	2p	7
6	4/5	2	2p	8
7	4/15	1	2p	9
8	2/3	2	2p	5
9	2/5	1	2p	10
10	8/15	2	2p	11
11	2/5	1	2p	12
12	2/3	1	2p	6
13	2/15	1	2p	13
14	2/5	2	2p	14
15	4/5	1	2p	15
$L = \ell$				
1	4/3	3	2s	1
2	4/3	4	2s	2

Table 3 (2nd page)

3	4/3	3	2s	3
4	2/3	5	2p	4
5	4/5	5	2p	7
6	2/5	6	2p	8
7	2/15	5	2p	9
8	2/3	7	2p	5
9	2/5	8	2p	10
10	8/15	7	2p	11
11	2/5	8	2p	12
12	2/3	3	2p	6
13	2/15	3	2p	13
14	2/5	4	2p	14
15	4/5	3	2p	15
16	-2/3	9	2p	5
17	-2/5	9	2p	10
18	4/15	9	2p	11
19	-2/3	9	2p	4
20	-2/5	9	2p	8
21	4/15	9	2p	9
$L=\ell-1$				
1	4/3	10	2s	1
2	4/3	11	2s	2

Table 3 (3rd page)

3	$4/3$	10	2s	3
4	$2/3$	12	2p	4
5	$4/5$	12	2p	7
6	$2/5$	13	2p	8
7	$2/15$	12	2p	9
8	$2/3$	14	2p	5
9	$2/5$	15	2p	10
10	$8/15$	14	2p	11
11	$2/5$	15	2p	12
12	$2/3$	16	2p	6
13	$2/15$	16	2p	13
14	$2/5$	17	2p	14
15	$4/5$	16	2p	15
16	$-2/3$	18	2p	5
17	$-2/5$	18	2p	10
18	$4/15$	18	2p	11
19	$-2/3$	18	2p	4
20	$-2/5$	18	2p	8
21	$4/15$	18	2p	9
22	$4/3$	19	2p	6
23	$4/15$	19	2p	13

Table 3 (4th page)

24	$4/3$	19	2p	4
25	$4/15$	19	2p	9
26	$2/3$	20	2p	6
27	$-4/15$	20	2p	13
28	$2/5$	20	2p	14
29	$2/3$	20	2p	5
30	$-4/15$	20	2p	11
31	$2/5$	20	2p	12

Table 4. The ℓ -dependent function $F_i(\ell)$ in the polarization potential $V_{pol}^L(r)$ in Eq. (34).

i	$F_i(\ell)$	i	$F_i(\ell)$
1	$\frac{(\ell+1)}{(2\ell+3)}$	11	$\frac{(2\ell^2+\ell-2)}{\ell(2\ell-1)(2\ell+1)}$
2	$\frac{1}{(2\ell+3)}$	12	$\frac{(4\ell^4+4\ell^3-3\ell^2-4\ell+6)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
3	$\frac{\ell(\ell+2)}{(\ell+1)(2\ell+3)}$	13	$\frac{(4\ell^3+8\ell^2+9\ell-15)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
4	$\frac{(\ell+3)}{(\ell+1)(2\ell+3)}$	14	$\frac{(4\ell^3+20\ell^2-13\ell-3)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
5	$\frac{\ell(\ell+3)}{(\ell+1)(2\ell+3)}$	15	$\frac{(4\ell^4+8\ell^3-9\ell^2+3)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
6	$\frac{(\ell+6)}{(\ell+1)(2\ell+3)}$	16	$\frac{(8\ell^4+4\ell^3-8\ell^2+3)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
7	$\frac{1}{(\ell+1)}$	17	$\frac{(8\ell^3+4\ell^2-6)}{\ell(2\ell-1)(2\ell+1)(2\ell+3)}$
8	$\frac{\ell}{(\ell+1)}$	18	$\frac{(2\ell-3)}{\ell(2\ell+1)(2\ell+3)}$
9	$\frac{\ell}{(\ell+1)(2\ell+3)}$	19	$\frac{1}{(2\ell+1)(2\ell+3)}$
10	$\frac{(2\ell^3-\ell^2-\ell+1)}{\ell(2\ell-1)(2\ell+1)}$	20	$\frac{(2\ell-1)}{(2\ell+1)(2\ell+3)}$

Table 5. Quadrature of the incident-electron energy k^2 in a.u.

For each region k_A^2 runs from k_B^2 in increments of δk^2 .

Region	k_A^2	δk^2	k_B^2
1	0.0	6.25×10^{-4}	0.025
2	0.025	1.25×10^{-3}	0.050
3	0.050	2.50×10^{-3}	0.100
4	0.100	5.0×10^{-3}	0.200
5	0.200	1.0×10^{-2}	1.200

Table 6. Absorption coefficients $\kappa(\lambda, T)$ of Eq. (12) in units of cm^5 . The wavelengths λ are in μm , and the temperature T in K. Numbers inside the parentheses indicate the power of 10.

$\lambda(\mu\text{m})$	T(K)					
	5000	10000	15000	20000	30000	50000
1.0	9.31(-40)	1.53(-39)	2.18(-39)	2.87(-39)	4.28(-39)	6.19(-39)
2.0	5.25(-39)	9.72(-39)	1.46(-38)	1.99(-38)	3.07(-38)	4.58(-38)
3.5	2.30(-38)	4.63(-38)	7.20(-38)	9.98(-38)	1.56(-37)	2.37(-37)
5.0	6.12(-38)	1.28(-37)	2.02(-37)	2.83(-37)	4.48(-37)	6.83(-37)
7.5	1.91(-37)	4.15(-37)	6.65(-37)	9.37(-37)	1.49(-36)	2.28(-36)
10.0	4.35(-37)	9.66(-37)	1.56(-36)	2.20(-36)	3.50(-36)	5.36(-36)
15.0	1.41(-36)	3.19(-36)	5.15(-36)	7.28(-36)	1.16(-35)	1.79(-35)
20.0	3.29(-36)	7.41(-36)	1.20(-35)	1.70(-35)	2.74(-35)	4.22(-35)
25.0	6.30(-36)	1.43(-35)	2.32(-35)	3.30(-35)	5.32(-35)	8.21(-35)
30.0	1.07(-35)	2.44(-35)	3.98(-35)	5.68(-35)	9.16(-35)	1.42(-34)

Table 7. Emissivity coefficients $J(\lambda, T)$ of Eq. (15) in units of $W\text{ cm}^3/\mu\text{m-steradian}$. The wavelengths λ are in units of μm , and the temperature T in K. Numbers inside the parentheses indicate the power of 10.

$\lambda(\mu\text{m})$	T(K)					
	5000	10000	15000	20000	30000	50000
1.0	6.22(-37)	4.32(-36)	9.94(-36)	1.66(-35)	3.10(-35)	5.24(-35)
2.0	4.63(-37)	1.76(-36)	3.37(-36)	5.17(-36)	8.92(-36)	1.44(-35)
3.5	2.30(-37)	6.96(-37)	1.24(-36)	1.84(-36)	3.09(-36)	4.88(-36)
5.0	1.31(-37)	3.66(-37)	6.37(-37)	9.35(-37)	1.55(-36)	2.43(-36)
7.5	6.53(-38)	1.72(-37)	2.94(-37)	4.28(-37)	7.02(-37)	1.10(-36)
10.0	3.89(-38)	9.97(-38)	1.69(-37)	2.44(-37)	3.98(-37)	6.18(-37)
15.0	1.88(-38)	4.57(-38)	7.60(-38)	1.09(-37)	1.77(-37)	2.75(-37)
20.0	1.06(-38)	2.57(-38)	4.27(-38)	6.13(-38)	9.95(-38)	1.55(-37)
25.0	6.99(-39)	1.65(-38)	2.73(-38)	3.92(-38)	6.37(-38)	9.90(-38)
30.0	4.77(-39)	1.14(-38)	1.89(-38)	2.72(-38)	4.42(-38)	6.88(-38)

Table 8. Comparison of the absorption coefficients $\kappa(\lambda, T)$ of Eq.(14) in cm^5 with other theoretical works (G and JW) and with the experimental values of Ref. [14]. Numbers inside the parentheses indicate the power of 10.

	$\lambda(\mu)$			
	2.0	3.5	5.0	10μ
Present (T = 10,000K)	9.72(-39)	4.63(-38)	1.28(-37)	9.66(-37)
G(Ref.[5]) (T = 10,000K)	7.13(-39)		8.97(-38)	6.68(-37)
JW(Ref.[7]) (T = 9,700K)	9.6(-39)	4.67(-38)	1.31(-37)	
Expt(Ref.[14]) (T=9,700K)	29.0(-39)	1.0(-38)	2.6(-37)	
	$\lambda(\mu)$			
	1.14	1.52	2.28	4.56
Present (T=5,000K)	1.2(-39)	2.5(-39)	7.3(-39)	4.9(-38)
JW(Ref.[7]) (T=5,040K)	1.09(-39)	2.28(-39)	6.60(-39)	4.38(-38)

Publications Resulting from this Contract

PUBLICATIONS

S. Chung and C. C. Lin, "Free-free transitions in collisions between slow electrons and neutral oxygen atoms", *Physical Review A* **51**, 1221 (1995).

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